tert-Butylhydroquinone

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Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (7	'5%)	Test (25%	Test (25%)		
Q2	RMSE	R2	RMSE	R2	RMSE		
0.89	0.25	0.88	0.26	0.75	0.38		

Model Results

Predicted value: 4.43 days

Global applicability domain: Outside

Local applicability domain index: 3.66e-01

Confidence level: 8.64e-01

Nearest Neighbors from the Training Set

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5-Methylindan Measured: 4.93 Predicted: 2.25 Image not found

Propylbenzene Measured: 24.3 Predicted: 4.02 Image not found

4-Ethyltoluene Measured: 24.3 Predicted: 3.95

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1,3-Diethylbenzene Measured: 88.3 Predicted: 5.36 Image not found

Ethylbenzene Measured: 120 Predicted: 6.21